WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 01:39 PM EDT

PDB ID	:	1YGU
Title	:	Crystal structure of the tandem phosphatase domains of RPTP CD45 with a pTyr peptide
Authors	:	Nam, H.; Poy, F.; Saito, H.; Frederick, C.A.
Deposited on	:	2005-01-05
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

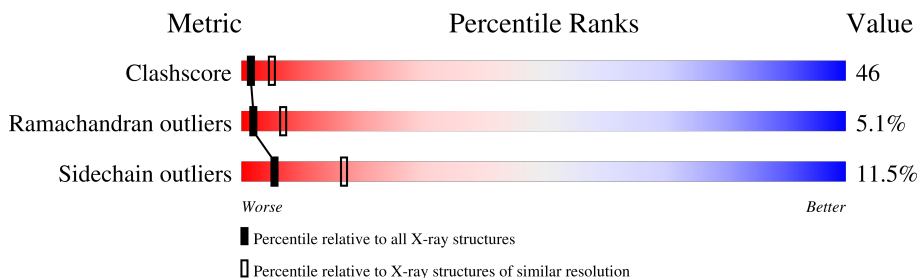|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		46
Ramachandran outliers		5.1%
Sidechain outliers		11.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	610	32% 51% 10% 6%
1	B	610	33% 51% 11% • 5%
2	C	4	25% 50% 25%
2	D	4	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTR	C	2004	X	-	-	-
2	PTR	D	2004	X	-	-	-

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9529 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Leukocyte common antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	Se	0	0	0
			4684	2983	815	866	7	13			
1	B	582	Total	C	N	O	S	Se	0	0	0
			4771	3033	835	883	7	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	MSE	MET	modified residue	UNP P08575
A	627	PRO	LEU	variant	UNP P08575
A	714	MSE	MET	modified residue	UNP P08575
A	725	MSE	MET	modified residue	UNP P08575
A	744	MSE	MET	modified residue	UNP P08575
A	828	SER	CYS	engineered mutation	UNP P08575
A	844	MSE	MET	modified residue	UNP P08575
A	870	MSE	MET	modified residue	UNP P08575
A	907	MSE	MET	modified residue	UNP P08575
A	999	MSE	MET	modified residue	UNP P08575
A	1007	MSE	MET	modified residue	UNP P08575
A	1024	MSE	MET	modified residue	UNP P08575
A	1035	MSE	MET	modified residue	UNP P08575
A	1115	MSE	MET	modified residue	UNP P08575
A	1184	LEU	PRO	variant	UNP P08575
A	1186	MSE	MET	modified residue	UNP P08575
B	603	MSE	MET	modified residue	UNP P08575
B	627	PRO	LEU	variant	UNP P08575
B	714	MSE	MET	modified residue	UNP P08575
B	725	MSE	MET	modified residue	UNP P08575
B	744	MSE	MET	modified residue	UNP P08575
B	828	SER	CYS	engineered mutation	UNP P08575
B	844	MSE	MET	modified residue	UNP P08575
B	870	MSE	MET	modified residue	UNP P08575
B	907	MSE	MET	modified residue	UNP P08575

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	999	MSE	MET	modified residue	UNP P08575
B	1007	MSE	MET	modified residue	UNP P08575
B	1024	MSE	MET	modified residue	UNP P08575
B	1035	MSE	MET	modified residue	UNP P08575
B	1115	MSE	MET	modified residue	UNP P08575
B	1184	LEU	PRO	variant	UNP P08575
B	1186	MSE	MET	modified residue	UNP P08575

- Molecule 2 is a protein called Polyoma Middle T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total 37	C 21	N 4	O 11	P 1	0	0	0
2	D	4	Total 37	C 21	N 4	O 11	P 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

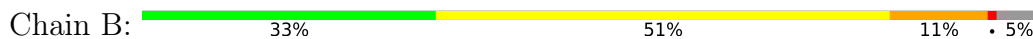| Chain	Residue	Modelled	Actual	Comment	Reference
C	2004	PTR	TYR	modified residue	UNP P03077
D	2004	PTR	TYR	modified residue	UNP P03077

3　Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
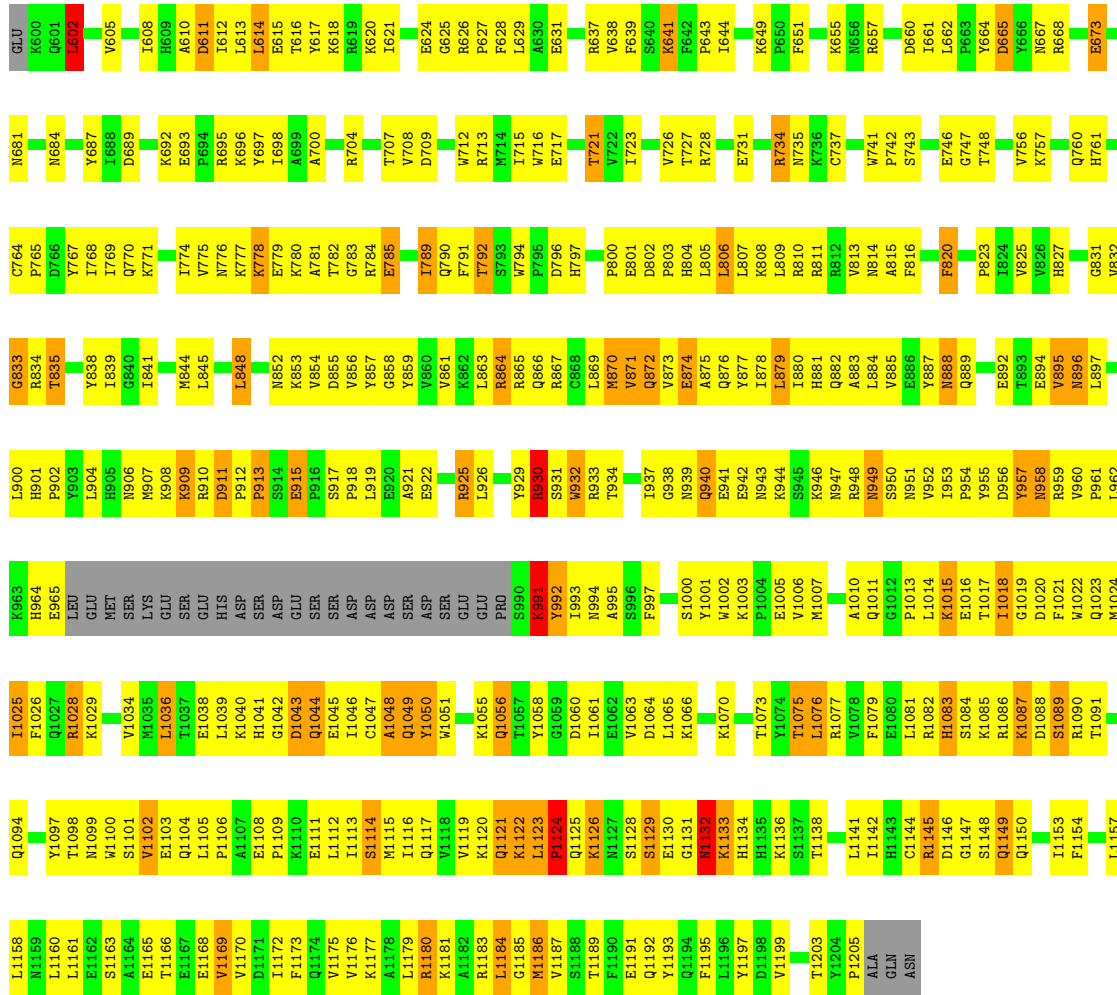
Note EDS was not executed.

• Molecule 1: Leukocyte common antigen
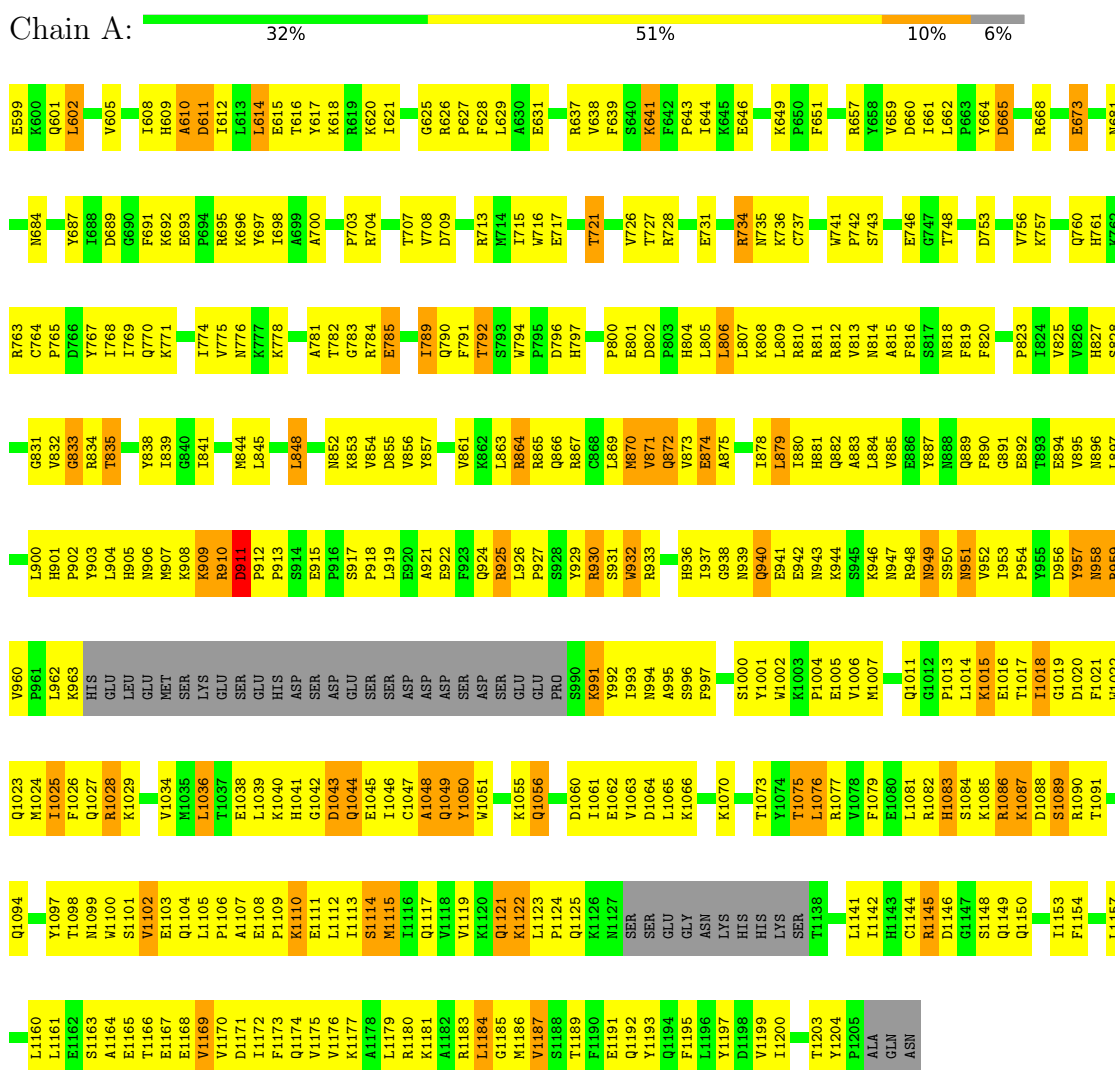
Chain A:

• Molecule 1: Leukocyte common antigen

Chain B:

• Molecule 2: Polyoma Middle T antigen

Chain C:

• Molecule 2: Polyoma Middle T antigen

Chain D:

4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.90Å 57.92Å 159.29Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	29.16 – 2.90	Depositor
% Data completeness (in resolution range)	92.9 (29.16-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9529	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PTR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.52	0/4779	0.72	1/6440 (0.0%)
1	B	0.52	0/4870	0.73	2/6562 (0.0%)
2	C	0.77	0/20	1.20	0/23
2	D	0.92	0/20	1.25	0/23
All	All	0.52	0/9689	0.73	3/13048 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	1	0
2	D	1	0
All	All	2	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1124	PRO	N-CA-C	5.53	126.47	112.10
1	B	602	LEU	N-CA-C	-5.19	96.99	111.00
1	A	781	ALA	N-CA-C	-5.09	97.25	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2004	PTR	CA
2	D	2004	PTR	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4684	0	4645	419	0
1	B	4771	0	4723	446	0
2	C	37	0	25	1	0
2	D	37	0	25	1	0
All	All	9529	0	9418	866	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (866) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:LEU:HD22	1:A:1186:MSE:HE3	1.27	1.14
1:B:844:MSE:HE3	1:B:854:VAL:HB	1.28	1.11
1:A:874:GLU:CD	1:A:874:GLU:H	1.50	1.08
1:A:844:MSE:HE3	1:A:854:VAL:HB	1.34	1.08
1:B:912:PRO:HB2	1:B:915:GLU:HG2	1.35	1.05
1:B:874:GLU:CD	1:B:874:GLU:H	1.61	1.03
1:A:911:ASP:HB3	1:A:912:PRO:HD3	1.39	1.00
1:A:1153:ILE:HD11	1:A:1192:GLN:HB3	1.46	0.98
1:B:911:ASP:HB2	1:B:912:PRO:HD3	1.48	0.93
1:B:962:LEU:HB3	1:B:991:LYS:HZ3	1.34	0.93
1:B:784:ARG:HD2	1:B:820:PHE:CZ	2.03	0.92
1:A:1040:LYS:HB3	1:A:1045:GLU:HA	1.51	0.91
1:B:1040:LYS:HB3	1:B:1045:GLU:HA	1.50	0.91
1:B:895:VAL:HG22	1:B:896:ASN:H	1.36	0.91
1:A:761:HIS:HD2	1:A:770:GLN:HE21	1.19	0.91
1:A:602:LEU:HD22	1:A:602:LEU:H	1.37	0.89
1:B:813:VAL:HG21	1:B:838:TYR:OH	1.73	0.89
1:B:1153:ILE:HD11	1:B:1192:GLN:HB3	1.51	0.89
1:B:844:MSE:CE	1:B:854:VAL:HB	2.01	0.89
1:A:873:VAL:HG12	1:A:875:ALA:H	1.40	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1083:HIS:CE1	1:B:1085:LYS:HE2	2.10	0.86
1:B:1044:GLN:H	1:B:1044:GLN:NE2	1.74	0.86
1:A:1115:MSE:O	1:A:1119:VAL:HG23	1.76	0.85
1:B:605:VAL:HG21	1:B:857:TYR:HB3	1.58	0.85
1:A:1179:LEU:HD22	1:A:1186:MSE:CE	2.06	0.84
1:B:777:LYS:NZ	1:B:781:ALA:HB3	1.93	0.83
1:A:813:VAL:HG21	1:A:838:TYR:OH	1.78	0.83
1:A:1022:TRP:HE1	1:A:1050:TYR:HB2	1.43	0.83
1:B:910:ARG:HD3	1:B:915:GLU:O	1.77	0.83
1:A:809:LEU:O	1:A:813:VAL:HG22	1.78	0.83
1:A:1018:ILE:HD11	1:A:1048:ALA:HB1	1.59	0.83
1:B:844:MSE:HE1	1:B:855:ASP:N	1.93	0.83
1:B:785:GLU:H	1:B:785:GLU:CD	1.81	0.82
1:A:940:GLN:HA	1:A:940:GLN:OE1	1.77	0.82
1:B:1018:ILE:HD11	1:B:1048:ALA:HB1	1.59	0.82
1:B:1082:ARG:HB3	1:B:1082:ARG:HH11	1.42	0.82
1:A:844:MSE:CE	1:A:854:VAL:HB	2.09	0.82
1:B:617:TYR:O	1:B:621:ILE:HG12	1.78	0.82
1:A:844:MSE:HE1	1:A:855:ASP:N	1.95	0.81
1:B:775:VAL:HG12	1:B:783:GLY:CA	2.11	0.81
1:A:929:TYR:O	1:A:932:TRP:HB2	1.81	0.80
1:B:1070:LYS:HG2	1:B:1075:THR:HB	1.63	0.80
1:B:1022:TRP:HE1	1:B:1050:TYR:HB2	1.46	0.80
1:B:605:VAL:HG21	1:B:857:TYR:CB	2.12	0.80
1:A:1082:ARG:HH11	1:A:1082:ARG:HB3	1.47	0.79
1:A:617:TYR:O	1:A:621:ILE:HG12	1.82	0.79
1:B:1082:ARG:HB3	1:B:1082:ARG:NH1	1.97	0.79
1:B:932:TRP:HZ3	1:B:957:TYR:CE2	2.01	0.79
1:A:605:VAL:HG21	1:A:857:TYR:HB3	1.65	0.78
1:A:911:ASP:HB3	1:A:912:PRO:CD	2.13	0.78
1:B:962:LEU:HB3	1:B:991:LYS:NZ	1.98	0.78
1:B:864:ARG:HG2	1:B:864:ARG:HH11	1.48	0.78
1:A:1083:HIS:CE1	1:A:1085:LYS:HE2	2.19	0.78
1:B:1002:TRP:HZ2	1:B:1166:THR:HG21	1.48	0.78
1:B:1115:MSE:O	1:B:1119:VAL:HG23	1.83	0.78
1:B:1087:LYS:HE3	1:B:1087:LYS:HA	1.66	0.78
1:A:910:ARG:HB3	1:A:917:SER:HA	1.64	0.77
1:A:864:ARG:HG2	1:A:864:ARG:HH11	1.47	0.77
1:B:929:TYR:HB3	1:B:932:TRP:HB2	1.66	0.77
1:B:1108:GLU:O	1:B:1111:GLU:HG2	1.85	0.76
1:A:785:GLU:CD	1:A:785:GLU:H	1.88	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:TYR:HB3	1:A:932:TRP:HB2	1.67	0.76
1:B:940:GLN:OE1	1:B:940:GLN:HA	1.83	0.76
1:A:932:TRP:HZ3	1:A:957:TYR:CE2	2.02	0.76
1:A:1082:ARG:HG2	1:A:1088:ASP:OD1	1.86	0.76
1:A:1097:TYR:HB2	1:A:1115:MSE:HE2	1.69	0.75
1:B:873:VAL:HG12	1:B:875:ALA:H	1.49	0.75
1:A:874:GLU:CD	1:A:874:GLU:N	2.32	0.75
1:A:910:ARG:HB3	1:A:917:SER:CA	2.16	0.75
1:B:608:ILE:HD12	1:B:608:ILE:H	1.50	0.75
1:A:1087:LYS:HE3	1:A:1087:LYS:HA	1.69	0.75
1:B:784:ARG:HD2	1:B:820:PHE:HZ	1.48	0.75
1:B:761:HIS:HD2	1:B:770:GLN:HE21	1.33	0.74
1:B:929:TYR:O	1:B:932:TRP:HB2	1.85	0.74
1:A:960:VAL:HA	1:A:997:PHE:HE2	1.53	0.74
1:B:949:ASN:HD22	1:B:950:SER:N	1.86	0.74
1:B:1126:LYS:NZ	1:B:1126:LYS:HB3	2.02	0.74
1:A:1063:VAL:HA	1:A:1081:LEU:HD23	1.70	0.74
1:A:660:ASP:HB3	1:A:661:ILE:HD12	1.70	0.74
1:A:1044:GLN:H	1:A:1044:GLN:NE2	1.85	0.74
1:B:775:VAL:HG12	1:B:783:GLY:HA2	1.70	0.73
1:A:605:VAL:HG21	1:A:857:TYR:CB	2.18	0.73
1:B:930:ARG:HE	1:B:930:ARG:HA	1.51	0.73
1:A:1002:TRP:HZ2	1:A:1166:THR:HG21	1.50	0.73
1:A:1022:TRP:NE1	1:A:1050:TYR:HB2	2.02	0.73
1:A:857:TYR:O	1:A:861:VAL:HG23	1.88	0.72
1:A:1142:ILE:HD13	1:A:1154:PHE:HD2	1.54	0.72
1:A:638:VAL:HG12	1:A:639:PHE:H	1.53	0.72
1:B:1038:GLU:OE1	1:B:1098:THR:HG23	1.88	0.72
1:A:1082:ARG:HB3	1:A:1082:ARG:NH1	2.03	0.72
1:A:911:ASP:O	1:A:913:PRO:CD	2.38	0.72
1:A:911:ASP:O	1:A:913:PRO:HD3	1.89	0.72
1:B:1160:LEU:HD22	1:B:1170:VAL:HG13	1.68	0.72
1:B:841:ILE:HG22	1:B:845:LEU:HD11	1.71	0.72
1:A:775:VAL:HG12	1:A:783:GLY:HA2	1.71	0.71
1:B:721:THR:HG22	1:B:785:GLU:O	1.90	0.71
1:B:1022:TRP:NE1	1:B:1050:TYR:HB2	2.05	0.71
1:A:721:THR:HG22	1:A:785:GLU:O	1.90	0.71
1:A:1070:LYS:HG2	1:A:1075:THR:HB	1.71	0.71
1:A:775:VAL:HG12	1:A:783:GLY:CA	2.20	0.71
1:A:617:TYR:CE2	1:A:621:ILE:HD13	2.25	0.71
1:A:841:ILE:HG22	1:A:845:LEU:HD11	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ASP:HB3	1:B:661:ILE:HD12	1.72	0.70
1:B:1063:VAL:HA	1:B:1081:LEU:HD23	1.74	0.70
1:A:963:LYS:HE3	1:A:1027:GLN:HB3	1.74	0.70
1:A:1153:ILE:CD1	1:A:1192:GLN:HB3	2.19	0.70
1:A:1038:GLU:OE1	1:A:1098:THR:HG23	1.91	0.70
1:A:949:ASN:HD22	1:A:950:SER:N	1.90	0.69
1:B:1120:LYS:HA	1:B:1123:LEU:HD12	1.74	0.69
1:A:864:ARG:HG2	1:A:864:ARG:NH1	2.07	0.69
1:A:1160:LEU:HD22	1:A:1170:VAL:HG13	1.74	0.69
1:A:930:ARG:HA	1:A:930:ARG:HE	1.58	0.69
1:B:947:ASN:ND2	1:B:992:TYR:OH	2.24	0.69
1:A:937:ILE:HG12	1:A:956:ASP:OD1	1.92	0.69
1:B:952:VAL:HG11	1:B:1146:ASP:HB2	1.75	0.68
1:B:874:GLU:O	1:B:878:ILE:HG13	1.92	0.68
1:A:1172:ILE:O	1:A:1176:VAL:HG23	1.92	0.68
1:B:954:PRO:HD3	1:B:994:ASN:OD1	1.92	0.68
1:A:1077:ARG:HE	1:A:1094:GLN:HE22	1.42	0.68
1:B:617:TYR:CE2	1:B:621:ILE:HD13	2.29	0.68
1:A:734:ARG:NH1	1:A:735:ASN:H	1.92	0.68
1:B:911:ASP:HB2	1:B:912:PRO:CD	2.24	0.67
1:A:599:GLU:HA	1:A:865:ARG:HH21	1.59	0.67
1:B:864:ARG:HG2	1:B:864:ARG:NH1	2.07	0.67
1:A:661:ILE:HD12	1:A:661:ILE:N	2.10	0.67
1:B:1063:VAL:HG12	1:B:1081:LEU:HD21	1.77	0.67
1:B:796:ASP:OD1	1:B:797:HIS:ND1	2.18	0.67
1:B:929:TYR:CE2	1:B:1181:LYS:HE3	2.30	0.67
1:B:1153:ILE:CD1	1:B:1192:GLN:HB3	2.22	0.67
1:B:809:LEU:O	1:B:813:VAL:HG22	1.94	0.66
1:A:806:LEU:HD23	1:A:841:ILE:HD11	1.77	0.66
1:A:909:LYS:HD2	1:A:909:LYS:C	2.15	0.66
1:A:949:ASN:HD22	1:A:949:ASN:C	1.99	0.66
1:A:608:ILE:HD12	1:A:608:ILE:H	1.59	0.66
1:B:1044:GLN:H	1:B:1044:GLN:HE21	1.42	0.66
1:B:932:TRP:CE3	1:B:933:ARG:HG3	2.30	0.66
1:B:948:ARG:HH12	1:B:1045:GLU:HG3	1.61	0.65
1:B:1142:ILE:HD13	1:B:1154:PHE:HD2	1.61	0.65
1:B:769:ILE:HG12	1:B:789:ILE:HG23	1.78	0.65
1:B:940:GLN:O	1:B:944:LYS:HG2	1.96	0.65
1:A:895:VAL:HG21	1:A:900:LEU:HA	1.76	0.65
1:A:909:LYS:HD2	1:A:909:LYS:O	1.97	0.65
1:A:952:VAL:HG11	1:A:1146:ASP:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:THR:O	1:B:620:LYS:HG2	1.96	0.65
1:A:940:GLN:O	1:A:944:LYS:HG2	1.95	0.65
1:A:1063:VAL:HA	1:A:1081:LEU:CD2	2.27	0.65
1:A:796:ASP:OD1	1:A:797:HIS:ND1	2.20	0.65
1:A:1061:ILE:C	1:A:1061:ILE:HD12	2.18	0.65
1:A:696:LYS:HD3	1:A:697:TYR:CZ	2.32	0.64
1:B:937:ILE:HG12	1:B:956:ASP:OD1	1.97	0.64
1:B:1183:ARG:HB3	1:B:1186:MSE:HE2	1.78	0.64
1:A:841:ILE:HG22	1:A:845:LEU:CD1	2.28	0.64
1:B:1061:ILE:HD12	1:B:1061:ILE:C	2.17	0.64
1:B:696:LYS:HD3	1:B:697:TYR:CZ	2.33	0.64
1:B:959:ARG:O	1:B:961:PRO:HD3	1.96	0.64
1:B:1014:LEU:C	1:B:1016:GLU:H	2.01	0.64
1:B:638:VAL:HG12	1:B:639:PHE:H	1.63	0.64
1:B:1098:THR:O	1:B:1100:TRP:N	2.30	0.64
1:A:704:ARG:H	1:A:707:THR:HB	1.61	0.64
1:A:731:GLU:OE2	1:A:796:ASP:HB2	1.98	0.64
1:A:1073:THR:HG22	1:A:1111:GLU:CD	2.18	0.64
1:B:1189:THR:HB	1:B:1191:GLU:OE1	1.97	0.64
1:A:1063:VAL:HG12	1:A:1081:LEU:HD21	1.79	0.64
1:B:704:ARG:H	1:B:707:THR:HB	1.63	0.64
1:A:1041:HIS:HB3	1:A:1044:GLN:HG2	1.78	0.64
1:B:731:GLU:OE2	1:B:796:ASP:HB2	1.98	0.64
1:A:878:ILE:O	1:A:882:GLN:HG3	1.97	0.64
1:B:962:LEU:HB3	1:B:991:LYS:HG2	1.79	0.64
1:B:794:TRP:NE1	1:B:834:ARG:HG2	2.13	0.63
1:A:951:ASN:O	1:A:1184:LEU:HD12	1.99	0.63
1:B:906:ASN:O	1:B:909:LYS:HG3	1.98	0.63
1:A:728:ARG:HG2	1:A:792:THR:HG22	1.80	0.63
1:B:958:ASN:O	1:B:997:PHE:HD2	1.81	0.63
1:B:1114:SER:HA	1:B:1117:GLN:HG2	1.80	0.63
1:A:1081:LEU:O	1:A:1089:SER:HA	1.99	0.63
1:B:1039:LEU:HD13	1:B:1049:GLN:HE21	1.64	0.63
1:A:1102:VAL:HB	1:A:1149:GLN:HE21	1.63	0.63
1:B:844:MSE:HE2	1:B:856:VAL:N	2.14	0.63
1:A:789:ILE:CG1	1:A:816:PHE:HE2	2.12	0.62
1:B:1039:LEU:HD22	1:B:1048:ALA:O	1.99	0.62
1:A:962:LEU:O	1:A:991:LYS:HB2	1.99	0.62
1:B:631:GLU:O	1:B:857:TYR:HE1	1.82	0.62
1:B:605:VAL:CG2	1:B:857:TYR:HB3	2.27	0.62
1:B:808:LYS:HE2	1:B:894:GLU:OE2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:ILE:HG22	1:B:845:LEU:CD1	2.29	0.62
1:A:1014:LEU:C	1:A:1016:GLU:H	2.02	0.62
1:B:1128:SER:O	1:B:1129:SER:HB2	1.99	0.62
1:B:1002:TRP:CZ2	1:B:1166:THR:HG21	2.33	0.62
1:B:774:ILE:O	1:B:783:GLY:HA2	2.00	0.62
1:B:942:GLU:N	1:B:942:GLU:OE1	2.33	0.62
1:A:958:ASN:O	1:A:997:PHE:HD2	1.83	0.61
1:B:912:PRO:HB2	1:B:915:GLU:CG	2.22	0.61
1:B:844:MSE:HE1	1:B:854:VAL:C	2.20	0.61
1:B:734:ARG:NH1	1:B:735:ASN:H	1.98	0.61
1:A:1179:LEU:HB3	1:A:1186:MSE:HG3	1.82	0.61
1:B:777:LYS:HZ2	1:B:781:ALA:HB3	1.63	0.61
1:B:1021:PHE:O	1:B:1025:ILE:HG23	2.00	0.61
1:A:631:GLU:O	1:A:857:TYR:HE1	1.83	0.61
1:A:844:MSE:HE2	1:A:856:VAL:N	2.16	0.61
1:A:873:VAL:HG12	1:A:875:ALA:N	2.13	0.61
1:A:1108:GLU:O	1:A:1111:GLU:HG2	2.00	0.61
1:B:1157:LEU:HD21	1:B:1199:VAL:HG21	1.83	0.61
1:B:938:GLY:HA2	1:B:992:TYR:CE1	2.36	0.61
1:A:922:GLU:N	1:A:925:ARG:HH21	1.99	0.61
1:A:1002:TRP:CZ2	1:A:1166:THR:HG21	2.35	0.61
1:B:626:ARG:N	1:B:627:PRO:CD	2.64	0.61
1:B:864:ARG:HD2	1:B:870:MSE:H	1.66	0.61
1:B:805:LEU:O	1:B:808:LYS:HB3	2.01	0.60
1:B:1199:VAL:O	1:B:1203:THR:HG23	2.01	0.60
1:A:605:VAL:CG2	1:A:857:TYR:HB3	2.31	0.60
1:A:1098:THR:O	1:A:1100:TRP:N	2.33	0.60
1:B:1121:GLN:O	1:B:1121:GLN:HG2	1.99	0.60
1:A:1039:LEU:HD13	1:A:1049:GLN:HG3	1.83	0.60
1:B:806:LEU:HD23	1:B:841:ILE:HD11	1.82	0.60
1:A:794:TRP:NE1	1:A:834:ARG:HG2	2.17	0.60
1:B:602:LEU:N	1:B:602:LEU:HD22	2.15	0.60
1:B:1161:LEU:O	1:B:1165:GLU:HG2	2.02	0.60
1:A:1077:ARG:NE	1:A:1094:GLN:HE22	1.99	0.60
1:B:942:GLU:HG2	1:B:943:ASN:ND2	2.16	0.60
1:B:1024:MSE:HE3	1:B:1141:LEU:HD11	1.83	0.60
1:B:881:HIS:O	1:B:885:VAL:HG23	2.01	0.60
1:B:991:LYS:H	1:B:991:LYS:HD3	1.65	0.60
1:A:626:ARG:N	1:A:627:PRO:CD	2.65	0.60
1:B:960:VAL:HA	1:B:997:PHE:HE2	1.67	0.59
1:A:760:GLN:HB2	1:A:771:LYS:HB2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:GLU:O	1:A:878:ILE:HG13	2.02	0.59
1:B:857:TYR:O	1:B:861:VAL:HG23	2.02	0.59
1:B:1040:LYS:CB	1:B:1045:GLU:HA	2.27	0.59
1:B:1183:ARG:O	1:B:1186:MSE:HG2	2.01	0.59
1:B:765:PRO:HG2	1:B:1001:TYR:CZ	2.37	0.59
1:B:844:MSE:HE2	1:B:856:VAL:CA	2.31	0.59
1:A:805:LEU:O	1:A:808:LYS:HB3	2.03	0.59
1:B:689:ASP:H	1:B:866:GLN:HE22	1.49	0.59
1:B:777:LYS:HD3	1:B:781:ALA:HB2	1.82	0.59
1:B:1160:LEU:HD23	1:B:1175:VAL:HG21	1.85	0.59
1:A:960:VAL:HA	1:A:997:PHE:CE2	2.36	0.59
1:B:1097:TYR:HB2	1:B:1115:MSE:HE2	1.85	0.59
1:A:932:TRP:CE3	1:A:933:ARG:HG3	2.37	0.59
1:B:1077:ARG:HE	1:B:1094:GLN:HE22	1.50	0.59
1:B:901:HIS:HB2	1:B:902:PRO:HD3	1.85	0.59
1:A:810:ARG:HD3	1:A:814:ASN:OD1	2.02	0.58
1:A:1039:LEU:HD13	1:A:1049:GLN:HE21	1.68	0.58
1:A:1101:SER:C	1:A:1103:GLU:H	2.06	0.58
1:A:769:ILE:HG12	1:A:789:ILE:HG23	1.85	0.58
1:B:778:LYS:HE2	1:B:778:LYS:HA	1.85	0.58
1:B:926:LEU:HD11	1:B:1193:TYR:CE1	2.38	0.58
1:B:1101:SER:C	1:B:1103:GLU:H	2.06	0.58
1:A:601:GLN:HA	1:A:601:GLN:OE1	2.04	0.58
1:B:1015:LYS:HA	1:B:1018:ILE:HG13	1.84	0.58
1:A:700:ALA:O	1:A:827:HIS:HB2	2.03	0.58
1:B:873:VAL:HG12	1:B:875:ALA:N	2.17	0.58
1:A:1039:LEU:HD22	1:A:1048:ALA:O	2.03	0.58
1:A:1121:GLN:O	1:A:1121:GLN:HG2	2.04	0.58
1:B:700:ALA:O	1:B:827:HIS:HB2	2.03	0.58
1:B:1013:PRO:HD2	1:B:1047:CYS:SG	2.44	0.58
1:A:1186:MSE:O	1:A:1187:VAL:C	2.42	0.58
1:B:904:LEU:HG	1:B:908:LYS:HE2	1.85	0.58
1:B:1063:VAL:HA	1:B:1081:LEU:CD2	2.33	0.58
1:B:1082:ARG:HG2	1:B:1088:ASP:OD1	2.03	0.58
1:A:638:VAL:HG12	1:A:639:PHE:N	2.19	0.58
1:B:992:TYR:C	1:B:992:TYR:CD2	2.77	0.57
1:B:1172:ILE:O	1:B:1176:VAL:HG23	2.04	0.57
1:B:615:GLU:HA	1:B:618:LYS:HB2	1.86	0.57
1:B:844:MSE:HE2	1:B:856:VAL:CG2	2.33	0.57
1:A:616:THR:O	1:A:620:LYS:HG2	2.05	0.57
1:A:794:TRP:CZ3	1:A:806:LEU:HD11	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:791:PHE:CD2	1:B:794:TRP:HB2	2.39	0.57
1:B:878:ILE:O	1:B:882:GLN:HG3	2.05	0.57
1:A:1189:THR:HB	1:A:1191:GLU:OE1	2.05	0.57
1:B:929:TYR:HD2	1:B:932:TRP:CD1	2.21	0.57
1:B:962:LEU:O	1:B:991:LYS:HD3	2.04	0.57
1:A:844:MSE:HE2	1:A:856:VAL:CA	2.34	0.57
1:B:926:LEU:HG	1:B:1173:PHE:CE1	2.39	0.57
1:A:602:LEU:HB2	1:A:857:TYR:OH	2.05	0.57
1:A:615:GLU:OE2	1:A:615:GLU:N	2.33	0.57
1:A:844:MSE:HE2	1:A:856:VAL:CG2	2.35	0.57
1:A:942:GLU:HG2	1:A:943:ASN:ND2	2.19	0.57
1:A:1015:LYS:NZ	1:A:1015:LYS:HB3	2.19	0.57
1:A:1157:LEU:HD21	1:A:1199:VAL:HG21	1.87	0.57
1:A:649:LYS:HD3	1:A:651:PHE:CZ	2.39	0.57
1:A:911:ASP:O	1:A:913:PRO:N	2.38	0.57
1:A:698:ILE:HG13	1:A:823:PRO:HB2	1.87	0.56
1:A:890:PHE:CE2	1:A:927:PRO:HD3	2.40	0.56
1:A:761:HIS:CD2	1:A:770:GLN:HE21	2.09	0.56
1:A:765:PRO:HG2	1:A:1001:TYR:CZ	2.40	0.56
1:A:804:HIS:CD2	1:A:1174:GLN:HG3	2.40	0.56
1:B:922:GLU:N	1:B:925:ARG:HH21	2.03	0.56
1:B:1011:GLN:HB2	1:B:1145:ARG:O	2.05	0.56
1:B:1148:SER:HB3	1:B:1185:GLY:C	2.26	0.56
1:B:1013:PRO:HG3	1:B:1050:TYR:CD2	2.40	0.56
1:B:1102:VAL:HB	1:B:1149:GLN:HE21	1.70	0.56
1:A:869:LEU:O	1:A:870:MSE:O	2.24	0.56
1:B:948:ARG:NH2	1:B:1047:CYS:HA	2.21	0.56
1:A:673:GLU:HG2	1:A:681:ASN:HB3	1.87	0.56
1:A:881:HIS:O	1:A:885:VAL:HG23	2.06	0.56
1:B:1179:LEU:HD22	1:B:1186:MSE:HE3	1.86	0.56
1:A:947:ASN:HD21	1:A:992:TYR:HE2	1.52	0.56
1:A:844:MSE:HE2	1:A:856:VAL:HG23	1.87	0.56
1:A:942:GLU:N	1:A:942:GLU:OE1	2.39	0.56
1:A:1015:LYS:HA	1:A:1018:ILE:HG13	1.88	0.56
1:A:734:ARG:NH1	1:A:735:ASN:N	2.53	0.56
1:B:831:GLY:HA2	1:B:835:THR:HG21	1.88	0.56
1:B:949:ASN:HD22	1:B:949:ASN:C	2.07	0.56
1:A:1014:LEU:C	1:A:1016:GLU:N	2.58	0.56
1:A:1044:GLN:H	1:A:1044:GLN:HE21	1.52	0.56
1:A:1097:TYR:CE2	1:A:1112:LEU:HD23	2.41	0.56
1:A:615:GLU:O	1:A:616:THR:C	2.44	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:GLY:HA3	1:A:953:ILE:CG2	2.36	0.55
1:A:1142:ILE:HD13	1:A:1154:PHE:CD2	2.40	0.55
1:B:728:ARG:HG2	1:B:792:THR:HG22	1.87	0.55
1:B:777:LYS:HZ3	1:B:781:ALA:HB3	1.66	0.55
1:B:897:LEU:HG	1:B:1168:GLU:HA	1.89	0.55
1:B:955:TYR:OH	1:B:1184:LEU:HD23	2.06	0.55
1:B:1049:GLN:O	1:B:1051:TRP:N	2.39	0.55
1:A:929:TYR:HD2	1:A:932:TRP:CD1	2.24	0.55
1:B:726:VAL:O	1:B:726:VAL:HG12	2.05	0.55
1:A:789:ILE:HD12	1:A:789:ILE:H	1.72	0.55
1:A:789:ILE:HG12	1:A:816:PHE:HE2	1.71	0.55
1:A:907:MSE:O	1:A:918:PRO:HD2	2.06	0.55
1:B:621:ILE:HG23	1:B:628:PHE:HE2	1.71	0.55
1:B:1073:THR:HG22	1:B:1111:GLU:CD	2.27	0.55
1:A:614:LEU:HD23	1:A:889:GLN:NE2	2.22	0.55
1:B:1160:LEU:CD2	1:B:1175:VAL:HG21	2.37	0.55
1:A:804:HIS:NE2	1:A:1174:GLN:HG3	2.22	0.55
1:A:870:MSE:O	1:A:871:VAL:C	2.45	0.55
1:A:1148:SER:HB3	1:A:1185:GLY:HA3	1.88	0.55
1:B:687:TYR:CG	1:B:695:ARG:HD2	2.41	0.55
1:B:874:GLU:CD	1:B:874:GLU:N	2.44	0.55
1:A:1014:LEU:O	1:A:1016:GLU:N	2.40	0.55
1:A:734:ARG:HH12	1:A:735:ASN:H	1.53	0.55
1:B:768:ILE:HG12	1:B:790:GLN:HB3	1.89	0.55
1:B:991:LYS:H	1:B:991:LYS:CD	2.20	0.55
1:B:1132:ASN:N	1:B:1132:ASN:HD22	2.04	0.55
1:A:962:LEU:HB3	1:A:991:LYS:CB	2.37	0.54
1:B:960:VAL:HA	1:B:997:PHE:CE2	2.42	0.54
1:A:962:LEU:HD11	1:A:1020:ASP:HB3	1.90	0.54
1:B:895:VAL:HG22	1:B:896:ASN:N	2.14	0.54
1:A:689:ASP:H	1:A:866:GLN:HE22	1.55	0.54
1:B:869:LEU:O	1:B:870:MSE:O	2.26	0.54
1:A:870:MSE:O	1:A:872:GLN:N	2.40	0.54
1:A:1046:ILE:HG23	1:A:1145:ARG:HG2	1.89	0.54
1:B:756:VAL:HG22	1:B:774:ILE:HG22	1.88	0.54
1:B:1157:LEU:HD21	1:B:1199:VAL:CG2	2.37	0.54
1:A:963:LYS:HZ2	1:A:963:LYS:HB2	1.73	0.54
1:B:713:ARG:O	1:B:717:GLU:HG3	2.06	0.54
1:A:929:TYR:HB3	1:A:932:TRP:CB	2.37	0.54
1:B:657:ARG:NH1	1:B:704:ARG:HG2	2.23	0.54
1:B:760:GLN:HB2	1:B:771:LYS:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:GLU:HG2	1:B:1169:VAL:HG22	1.89	0.54
1:B:1014:LEU:C	1:B:1016:GLU:N	2.57	0.54
1:A:948:ARG:HH12	1:A:1045:GLU:HG3	1.72	0.54
1:A:1114:SER:HA	1:A:1117:GLN:HG2	1.90	0.54
1:B:870:MSE:O	1:B:871:VAL:C	2.44	0.54
1:B:929:TYR:HE2	1:B:1181:LYS:HE3	1.71	0.54
1:B:743:SER:OG	1:B:746:GLU:HG2	2.08	0.54
1:B:844:MSE:HE2	1:B:856:VAL:HG23	1.89	0.54
1:B:929:TYR:O	1:B:930:ARG:C	2.47	0.54
1:B:946:LYS:C	1:B:947:ASN:HD22	2.11	0.54
1:B:962:LEU:CB	1:B:991:LYS:HG2	2.36	0.54
1:B:1113:ILE:HG13	1:B:1203:THR:HG21	1.88	0.54
1:A:615:GLU:HA	1:A:618:LYS:HB2	1.89	0.54
1:A:901:HIS:HB2	1:A:902:PRO:HD3	1.89	0.54
1:B:649:LYS:HD3	1:B:651:PHE:CZ	2.42	0.54
1:B:789:ILE:HD12	1:B:789:ILE:H	1.73	0.54
1:B:810:ARG:HD3	1:B:814:ASN:OD1	2.08	0.54
1:B:909:LYS:HD2	1:B:909:LYS:O	2.08	0.54
1:B:929:TYR:HB3	1:B:932:TRP:CB	2.36	0.54
1:A:1157:LEU:HD21	1:A:1199:VAL:CG2	2.38	0.54
1:B:1081:LEU:O	1:B:1089:SER:HA	2.08	0.54
1:A:791:PHE:CD2	1:A:794:TRP:HB2	2.42	0.53
1:A:918:PRO:O	1:A:921:ALA:HB3	2.08	0.53
1:B:1063:VAL:HG12	1:B:1081:LEU:CD2	2.39	0.53
1:A:599:GLU:HA	1:A:865:ARG:NH2	2.23	0.53
1:A:831:GLY:HA2	1:A:835:THR:HG21	1.89	0.53
1:B:1025:ILE:HD11	1:B:1081:LEU:CD1	2.38	0.53
1:A:768:ILE:HG12	1:A:790:GLN:HB3	1.90	0.53
1:A:929:TYR:CE2	1:A:1181:LYS:HE3	2.43	0.53
1:A:1179:LEU:CD2	1:A:1186:MSE:HE3	2.18	0.53
1:A:726:VAL:HG12	1:A:726:VAL:O	2.07	0.53
1:A:774:ILE:O	1:A:783:GLY:HA2	2.08	0.53
1:A:1021:PHE:O	1:A:1025:ILE:HG23	2.08	0.53
1:A:1046:ILE:HG23	1:A:1145:ARG:HE	1.74	0.53
1:B:929:TYR:HB3	1:B:932:TRP:CG	2.44	0.53
1:B:1018:ILE:HG23	1:B:1050:TYR:HA	1.89	0.53
1:B:1070:LYS:HG2	1:B:1075:THR:CB	2.35	0.53
1:B:1105:LEU:O	1:B:1106:PRO:C	2.47	0.53
1:B:775:VAL:HG12	1:B:783:GLY:HA3	1.88	0.53
1:B:1061:ILE:HD12	1:B:1061:ILE:O	2.08	0.53
1:A:869:LEU:O	1:A:869:LEU:HG	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1041:HIS:HB3	1:B:1044:GLN:HG2	1.91	0.53
1:A:1018:ILE:HG23	1:A:1050:TYR:HA	1.91	0.53
1:B:615:GLU:O	1:B:616:THR:C	2.47	0.53
1:B:794:TRP:CZ3	1:B:806:LEU:HD11	2.44	0.53
1:B:906:ASN:C	1:B:908:LYS:H	2.12	0.53
1:B:894:GLU:O	1:B:895:VAL:O	2.27	0.53
1:B:614:LEU:HD22	1:B:885:VAL:CG1	2.39	0.53
1:B:844:MSE:CE	1:B:856:VAL:N	2.72	0.53
1:B:855:ASP:OD2	1:B:858:GLY:HA3	2.09	0.53
1:B:911:ASP:CB	1:B:912:PRO:HD3	2.30	0.53
1:B:1014:LEU:O	1:B:1016:GLU:N	2.42	0.53
1:A:1144:CYS:O	1:A:1145:ARG:C	2.46	0.52
1:A:1203:THR:O	1:A:1204:TYR:CD1	2.62	0.52
1:B:621:ILE:O	1:B:625:GLY:N	2.42	0.52
1:B:707:THR:HG22	1:B:707:THR:O	2.10	0.52
1:B:1186:MSE:O	1:B:1187:VAL:C	2.46	0.52
1:A:611:ASP:OD1	1:A:612:ILE:HG23	2.10	0.52
1:A:960:VAL:HG22	1:A:997:PHE:CE2	2.45	0.52
1:B:661:ILE:HD12	1:B:661:ILE:N	2.23	0.52
1:B:820:PHE:CD1	1:B:820:PHE:N	2.77	0.52
1:B:906:ASN:C	1:B:908:LYS:N	2.62	0.52
1:B:908:LYS:O	1:B:917:SER:HB2	2.09	0.52
1:B:1025:ILE:HD12	1:B:1025:ILE:O	2.09	0.52
1:B:1028:ARG:HG3	1:B:1028:ARG:HH11	1.74	0.52
1:B:1126:LYS:HB3	1:B:1126:LYS:HZ2	1.70	0.52
1:A:621:ILE:HG23	1:A:628:PHE:HE2	1.75	0.52
1:A:1049:GLN:O	1:A:1051:TRP:N	2.43	0.52
1:A:930:ARG:HG3	1:A:931:SER:N	2.24	0.52
1:B:608:ILE:HD12	1:B:608:ILE:N	2.19	0.52
1:B:930:ARG:HG3	1:B:931:SER:N	2.25	0.52
1:B:1136:LYS:HD2	1:B:1136:LYS:N	2.25	0.52
1:A:844:MSE:HE1	1:A:854:VAL:C	2.29	0.52
1:A:1040:LYS:CB	1:A:1045:GLU:HA	2.33	0.52
1:A:1088:ASP:O	1:A:1089:SER:C	2.47	0.52
1:B:1088:ASP:O	1:B:1089:SER:C	2.48	0.52
1:A:715:ILE:CD1	1:A:825:VAL:HG21	2.40	0.52
1:B:741:TRP:HB2	1:B:742:PRO:HD2	1.92	0.52
1:B:922:GLU:CA	1:B:925:ARG:HH21	2.23	0.52
1:A:812:ARG:O	1:A:815:ALA:HB3	2.09	0.52
1:B:791:PHE:CE2	1:B:794:TRP:HB2	2.44	0.52
1:B:806:LEU:HA	1:B:809:LEU:CD2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:LEU:HD23	1:A:1175:VAL:HG21	1.92	0.51
1:A:608:ILE:O	1:A:853:LYS:HA	2.11	0.51
1:A:1013:PRO:HG3	1:A:1050:TYR:CD2	2.44	0.51
1:B:618:LYS:O	1:B:621:ILE:HG13	2.10	0.51
1:B:897:LEU:HG	1:B:1168:GLU:CA	2.40	0.51
1:A:743:SER:OG	1:A:746:GLU:HG2	2.10	0.51
1:A:880:ILE:O	1:A:883:ALA:HB3	2.09	0.51
1:A:1055:LYS:HE3	1:A:1062:GLU:OE1	2.11	0.51
1:B:895:VAL:HG21	1:B:900:LEU:HA	1.92	0.51
1:B:929:TYR:OH	1:B:1177:LYS:HE2	2.10	0.51
1:B:1017:THR:O	1:B:1019:GLY:N	2.44	0.51
1:B:1083:HIS:NE2	1:B:1085:LYS:HE2	2.25	0.51
1:A:994:ASN:OD1	1:A:1183:ARG:NH2	2.44	0.51
1:B:649:LYS:HD3	1:B:651:PHE:HZ	1.76	0.51
1:B:907:MSE:O	1:B:918:PRO:HD2	2.11	0.51
1:B:953:ILE:HA	1:B:994:ASN:HD21	1.75	0.51
1:A:614:LEU:HD22	1:A:885:VAL:CG1	2.41	0.51
1:A:929:TYR:HB3	1:A:932:TRP:CG	2.46	0.51
1:A:1011:GLN:HB2	1:A:1145:ARG:O	2.10	0.51
1:B:901:HIS:CB	1:B:902:PRO:HD3	2.40	0.51
1:B:1044:GLN:HE21	1:B:1044:GLN:N	2.08	0.51
1:B:1077:ARG:NE	1:B:1094:GLN:HE22	2.08	0.51
1:A:764:CYS:HB3	1:A:765:PRO:CD	2.40	0.51
1:A:1017:THR:C	1:A:1019:GLY:N	2.64	0.51
1:B:1192:GLN:O	1:B:1195:PHE:HB3	2.11	0.51
1:B:734:ARG:HH12	1:B:735:ASN:H	1.57	0.51
1:B:1142:ILE:HD13	1:B:1154:PHE:CD2	2.45	0.51
1:A:657:ARG:NH2	1:A:737:CYS:HA	2.25	0.50
1:A:818:ASN:O	1:A:820:PHE:N	2.44	0.50
1:A:748:THR:OG1	1:A:757:LYS:HG3	2.11	0.50
1:A:910:ARG:HD3	1:A:915:GLU:O	2.11	0.50
1:A:1153:ILE:HD13	1:A:1187:VAL:HG22	1.93	0.50
1:B:964:HIS:O	1:B:965:GLU:C	2.48	0.50
1:A:1026:PHE:CE2	1:A:1090:ARG:NH1	2.79	0.50
1:B:684:ASN:OD1	1:B:867:ARG:NH2	2.38	0.50
1:B:1101:SER:HB3	1:B:1103:GLU:OE1	2.11	0.50
1:B:801:GLU:CD	1:B:801:GLU:H	2.15	0.50
1:B:1141:LEU:HD23	1:B:1142:ILE:N	2.27	0.50
1:A:801:GLU:OE1	1:A:805:LEU:CD1	2.60	0.50
1:B:1087:LYS:HE3	1:B:1087:LYS:CA	2.40	0.50
1:A:599:GLU:CA	1:A:865:ARG:HH21	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LYS:O	1:A:643:PRO:HD3	2.11	0.50
1:A:791:PHE:CE2	1:A:794:TRP:HB2	2.47	0.50
1:A:1113:ILE:HG13	1:A:1203:THR:HG21	1.93	0.50
1:B:608:ILE:H	1:B:608:ILE:CD1	2.23	0.50
1:B:1039:LEU:HD13	1:B:1049:GLN:HG3	1.93	0.50
1:A:947:ASN:ND2	1:A:994:ASN:HD22	2.09	0.50
1:A:1004:PRO:O	1:A:1006:VAL:HG23	2.11	0.50
1:A:1029:LYS:HA	1:A:1090:ARG:NH2	2.27	0.50
1:A:713:ARG:O	1:A:717:GLU:HG3	2.11	0.50
1:A:716:TRP:O	1:A:784:ARG:NH2	2.44	0.50
1:B:698:ILE:HG13	1:B:823:PRO:HB2	1.94	0.50
1:B:768:ILE:O	1:B:768:ILE:HG13	2.12	0.50
1:B:873:VAL:CG1	1:B:875:ALA:H	2.23	0.50
1:A:904:LEU:HG	1:A:908:LYS:HE2	1.94	0.50
1:A:1014:LEU:O	1:A:1017:THR:N	2.43	0.50
1:B:638:VAL:HG12	1:B:639:PHE:N	2.25	0.50
1:B:901:HIS:NE2	1:B:1205:PRO:HA	2.27	0.50
1:B:1000:SER:HB3	1:B:1005:GLU:O	2.12	0.50
1:B:1131:GLY:O	1:B:1132:ASN:HB3	2.12	0.50
1:A:926:LEU:HG	1:A:1173:PHE:CE1	2.47	0.49
1:B:803:PRO:O	1:B:807:LEU:HD13	2.12	0.49
1:A:684:ASN:OD1	1:A:867:ARG:NH2	2.40	0.49
1:B:712:TRP:CE2	1:B:756:VAL:HG21	2.47	0.49
1:B:1043:ASP:HB2	1:B:1044:GLN:NE2	2.28	0.49
1:A:1105:LEU:O	1:A:1106:PRO:C	2.51	0.49
1:B:716:TRP:O	1:B:784:ARG:NH2	2.44	0.49
1:B:1020:ASP:HA	1:B:1023:GLN:OE1	2.13	0.49
1:A:657:ARG:NH1	1:A:704:ARG:HG2	2.27	0.49
1:A:922:GLU:CA	1:A:925:ARG:HH21	2.25	0.49
1:A:1017:THR:O	1:A:1019:GLY:N	2.45	0.49
1:B:613:LEU:HD23	1:B:888:ASN:OD1	2.12	0.49
1:B:644:ILE:HG12	1:B:664:TYR:HA	1.94	0.49
1:B:687:TYR:CD2	1:B:695:ARG:HD2	2.48	0.49
1:B:697:TYR:CE1	1:B:839:ILE:HG23	2.47	0.49
1:B:929:TYR:CE2	1:B:1181:LYS:HG3	2.47	0.49
1:A:897:LEU:HG	1:A:1168:GLU:O	2.13	0.49
1:A:962:LEU:HB3	1:A:991:LYS:HB3	1.95	0.49
1:B:1002:TRP:O	1:B:1005:GLU:HG2	2.13	0.49
1:B:1144:CYS:O	1:B:1145:ARG:C	2.51	0.49
1:A:599:GLU:HB3	1:A:865:ARG:NH2	2.28	0.49
1:A:844:MSE:CE	1:A:856:VAL:N	2.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:LEU:HD23	1:A:1142:ILE:N	2.27	0.49
1:A:1160:LEU:CD2	1:A:1175:VAL:HG21	2.42	0.49
1:B:1014:LEU:O	1:B:1017:THR:N	2.42	0.49
1:B:1083:HIS:CE1	1:B:1085:LYS:HB3	2.47	0.49
1:A:649:LYS:HD3	1:A:651:PHE:HZ	1.75	0.49
1:A:764:CYS:HB3	1:A:765:PRO:HD2	1.95	0.49
1:A:801:GLU:OE1	1:A:805:LEU:HD11	2.13	0.49
1:B:870:MSE:O	1:B:872:GLN:N	2.45	0.49
1:B:1187:VAL:HG13	1:B:1192:GLN:HB2	1.95	0.49
1:A:926:LEU:HD11	1:A:1193:TYR:CE1	2.48	0.49
1:B:813:VAL:C	1:B:815:ALA:H	2.16	0.49
1:B:848:LEU:HD23	1:B:852:ASN:HA	1.93	0.49
1:B:1015:LYS:NZ	1:B:1015:LYS:HB3	2.28	0.49
1:B:1097:TYR:OH	1:B:1111:GLU:HG3	2.13	0.49
1:A:806:LEU:HD23	1:A:841:ILE:CD1	2.42	0.49
1:A:1082:ARG:NH1	1:A:1082:ARG:CB	2.75	0.49
1:A:801:GLU:CD	1:A:801:GLU:H	2.15	0.49
1:B:707:THR:O	1:B:707:THR:CG2	2.61	0.49
1:B:734:ARG:NH1	1:B:735:ASN:N	2.60	0.48
1:B:806:LEU:HD23	1:B:841:ILE:CD1	2.43	0.48
1:A:707:THR:O	1:A:707:THR:HG22	2.13	0.48
1:A:900:LEU:HD21	1:A:1200:ILE:HG22	1.95	0.48
1:A:993:ILE:HD13	1:A:1024:MSE:SE	2.62	0.48
1:B:932:TRP:CD2	1:B:933:ARG:HG3	2.48	0.48
1:B:954:PRO:HD3	1:B:994:ASN:CG	2.34	0.48
1:B:1082:ARG:NH1	1:B:1082:ARG:CB	2.70	0.48
1:A:939:ASN:HA	1:A:944:LYS:HD3	1.95	0.48
1:B:1025:ILE:HD11	1:B:1081:LEU:HD11	1.95	0.48
1:B:1034:VAL:HG12	1:B:1036:LEU:HD13	1.96	0.48
1:A:889:GLN:NE2	1:A:889:GLN:HA	2.28	0.48
1:A:1171:ASP:OD1	1:A:1174:GLN:HB2	2.14	0.48
1:A:1192:GLN:O	1:A:1195:PHE:HB3	2.13	0.48
1:B:910:ARG:HB2	1:B:915:GLU:O	2.12	0.48
1:B:1049:GLN:C	1:B:1051:TRP:H	2.16	0.48
1:A:707:THR:O	1:A:707:THR:CG2	2.60	0.48
1:A:1087:LYS:HE3	1:A:1087:LYS:CA	2.42	0.48
1:B:764:CYS:HB3	1:B:765:PRO:HD2	1.95	0.48
1:B:800:PRO:HD2	1:B:879:LEU:HD11	1.96	0.48
1:B:801:GLU:OE1	1:B:805:LEU:CD1	2.61	0.48
1:A:768:ILE:O	1:A:768:ILE:HG13	2.13	0.48
1:A:854:VAL:HG23	1:A:854:VAL:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ARG:HH21	1:A:1184:LEU:HD21	1.78	0.48
1:A:958:ASN:O	1:A:959:ARG:C	2.51	0.48
1:A:897:LEU:CD1	1:A:1168:GLU:HA	2.44	0.48
1:B:1046:ILE:HG23	1:B:1145:ARG:HG2	1.95	0.48
1:A:1025:ILE:HD11	1:A:1081:LEU:CD1	2.43	0.48
1:A:932:TRP:CD2	1:A:933:ARG:HG3	2.49	0.48
1:A:1001:TYR:CE1	1:A:1163:SER:HB3	2.49	0.48
1:A:1063:VAL:HG12	1:A:1081:LEU:CD2	2.44	0.48
1:A:1083:HIS:O	1:A:1085:LYS:N	2.47	0.48
1:B:844:MSE:HE2	1:B:856:VAL:HA	1.95	0.48
1:B:1045:GLU:HG3	1:B:1045:GLU:O	2.14	0.48
1:A:767:TYR:HA	1:A:790:GLN:O	2.14	0.48
1:A:946:LYS:C	1:A:947:ASN:HD22	2.17	0.48
1:A:1039:LEU:CD1	1:A:1049:GLN:HG3	2.43	0.48
1:B:839:ILE:HD12	1:B:870:MSE:HE1	1.95	0.47
1:B:929:TYR:CD2	1:B:1181:LYS:HG3	2.49	0.47
1:A:608:ILE:HD12	1:A:608:ILE:N	2.28	0.47
1:A:692:LYS:O	1:A:693:GLU:C	2.52	0.47
1:B:922:GLU:HG2	1:B:1173:PHE:CD1	2.49	0.47
1:A:621:ILE:O	1:A:625:GLY:N	2.46	0.47
1:A:848:LEU:HD23	1:A:852:ASN:HA	1.96	0.47
1:A:958:ASN:O	1:A:959:ARG:O	2.32	0.47
1:B:611:ASP:OD1	1:B:612:ILE:HG23	2.15	0.47
1:B:1017:THR:C	1:B:1019:GLY:N	2.65	0.47
1:B:1046:ILE:HG23	1:B:1145:ARG:HE	1.79	0.47
1:B:1131:GLY:O	1:B:1132:ASN:CB	2.62	0.47
1:A:929:TYR:OH	1:A:1177:LYS:HE2	2.15	0.47
1:A:1097:TYR:CD2	1:A:1112:LEU:HD23	2.48	0.47
1:B:657:ARG:NH2	1:B:737:CYS:HA	2.29	0.47
1:B:692:LYS:O	1:B:693:GLU:C	2.53	0.47
1:A:668:ARG:NH1	1:A:681:ASN:OD1	2.47	0.47
1:A:863:LEU:HB3	1:A:870:MSE:HG3	1.95	0.47
1:A:996:SER:OG	1:A:1183:ARG:NE	2.46	0.47
1:A:1160:LEU:O	1:A:1164:ALA:HB2	2.15	0.47
1:B:922:GLU:HA	1:B:925:ARG:HH21	1.79	0.47
1:B:1028:ARG:HD2	1:B:1028:ARG:N	2.30	0.47
1:A:949:ASN:C	1:A:949:ASN:ND2	2.65	0.47
1:A:1061:ILE:HD12	1:A:1061:ILE:O	2.15	0.47
1:B:1132:ASN:N	1:B:1132:ASN:ND2	2.63	0.47
1:A:602:LEU:HD22	1:A:602:LEU:N	2.18	0.47
1:B:1055:LYS:O	1:B:1055:LYS:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PRO:HD2	1:A:879:LEU:HD11	1.96	0.46
1:A:962:LEU:HD12	1:A:993:ILE:HB	1.96	0.46
1:A:1000:SER:HB3	1:A:1005:GLU:O	2.15	0.46
1:A:1161:LEU:O	1:A:1165:GLU:HG2	2.14	0.46
1:B:1040:LYS:HA	1:B:1046:ILE:HG13	1.97	0.46
1:A:734:ARG:CZ	1:A:734:ARG:HA	2.45	0.46
1:A:863:LEU:C	1:A:865:ARG:H	2.18	0.46
1:A:896:ASN:ND2	1:A:1169:VAL:HG23	2.30	0.46
1:A:925:ARG:HE	1:A:925:ARG:HB2	1.61	0.46
1:A:618:LYS:O	1:A:621:ILE:HG13	2.15	0.46
1:A:657:ARG:NH1	1:A:703:PRO:O	2.45	0.46
1:B:689:ASP:N	1:B:866:GLN:HE22	2.13	0.46
1:A:844:MSE:HE2	1:A:856:VAL:HA	1.97	0.46
1:A:922:GLU:HG2	1:A:1173:PHE:CD1	2.50	0.46
1:B:708:VAL:HG23	1:B:709:ASP:N	2.30	0.46
1:B:767:TYR:HA	1:B:790:GLN:O	2.15	0.46
1:B:1141:LEU:HD23	1:B:1141:LEU:C	2.36	0.46
1:A:646:GLU:HG3	1:A:668:ARG:NH2	2.30	0.46
1:A:775:VAL:HG12	1:A:783:GLY:HA3	1.97	0.46
1:A:929:TYR:O	1:A:930:ARG:C	2.54	0.46
1:B:764:CYS:HB3	1:B:765:PRO:CD	2.45	0.46
1:B:863:LEU:C	1:B:865:ARG:H	2.19	0.46
1:B:938:GLY:HA3	1:B:953:ILE:CG2	2.46	0.46
1:A:839:ILE:HD12	1:A:870:MSE:HE1	1.97	0.46
1:A:940:GLN:OE1	1:A:940:GLN:CA	2.55	0.46
1:A:1064:ASP:OD2	1:A:1066:LYS:HE2	2.16	0.46
1:B:668:ARG:NH1	1:B:681:ASN:OD1	2.49	0.46
1:B:831:GLY:O	1:B:867:ARG:HD3	2.15	0.46
1:A:958:ASN:N	1:A:958:ASN:HD22	2.13	0.46
1:A:1170:VAL:HG12	1:A:1172:ILE:HG13	1.98	0.46
1:B:614:LEU:HG	1:B:889:GLN:HE22	1.79	0.46
1:B:618:LYS:HA	1:B:621:ILE:HD11	1.98	0.46
1:A:1020:ASP:HA	1:A:1023:GLN:OE1	2.16	0.46
1:B:615:GLU:OE2	1:B:615:GLU:N	2.41	0.46
1:B:1112:LEU:O	1:B:1116:ILE:HG13	2.16	0.46
1:A:1101:SER:C	1:A:1103:GLU:N	2.70	0.46
1:B:1070:LYS:HG2	1:B:1075:THR:CG2	2.46	0.46
1:B:904:LEU:HD13	1:B:1197:TYR:CD1	2.51	0.45
1:A:958:ASN:C	1:A:959:ARG:O	2.54	0.45
1:B:864:ARG:HH11	1:B:864:ARG:CG	2.23	0.45
1:B:918:PRO:O	1:B:921:ALA:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:HIS:CB	1:A:902:PRO:HD3	2.46	0.45
1:A:1025:ILE:HD12	1:A:1025:ILE:O	2.16	0.45
1:B:673:GLU:HG2	1:B:681:ASN:HB3	1.98	0.45
1:B:1041:HIS:O	1:B:1043:ASP:N	2.49	0.45
1:A:1153:ILE:HD11	1:A:1192:GLN:CB	2.30	0.45
1:B:1082:ARG:HG3	1:B:1089:SER:HA	1.99	0.45
1:B:1160:LEU:HD21	1:B:1172:ILE:HA	1.98	0.45
1:A:741:TRP:HB2	1:A:742:PRO:HD2	1.97	0.45
1:A:1045:GLU:HG3	1:A:1045:GLU:O	2.16	0.45
1:A:1097:TYR:CD1	1:A:1115:MSE:HG3	2.52	0.45
1:B:1022:TRP:CZ2	1:B:1050:TYR:HD1	2.34	0.45
1:B:1026:PHE:CE2	1:B:1090:ARG:NH1	2.85	0.45
1:B:1097:TYR:CE2	1:B:1112:LEU:HD23	2.51	0.45
1:A:1022:TRP:CZ2	1:A:1050:TYR:HD1	2.35	0.45
1:B:605:VAL:HG21	1:B:857:TYR:HB2	1.97	0.45
1:B:831:GLY:C	1:B:835:THR:HG21	2.37	0.45
1:B:832:VAL:HG23	1:B:833:GLY:N	2.31	0.45
1:B:1083:HIS:O	1:B:1085:LYS:N	2.49	0.45
1:A:864:ARG:HD2	1:A:870:MSE:H	1.81	0.45
1:B:608:ILE:O	1:B:853:LYS:HA	2.17	0.45
1:B:880:ILE:O	1:B:883:ALA:HB3	2.17	0.45
1:B:641:LYS:O	1:B:643:PRO:HD3	2.17	0.45
1:B:1101:SER:C	1:B:1103:GLU:N	2.71	0.45
1:B:1170:VAL:HG12	1:B:1172:ILE:HG13	1.98	0.45
2:C:2004:PTR:O	2:C:2005:SER:HB2	2.16	0.45
1:A:643:PRO:O	1:A:665:ASP:HB2	2.17	0.45
1:A:756:VAL:HG22	1:A:774:ILE:HG22	1.99	0.45
1:A:938:GLY:HA3	1:A:953:ILE:HG21	1.99	0.45
1:B:859:TYR:CE1	1:B:863:LEU:HD11	2.52	0.45
1:B:1014:LEU:HB3	1:B:1016:GLU:HG2	1.98	0.45
1:A:618:LYS:HA	1:A:621:ILE:HD11	1.99	0.45
1:A:813:VAL:C	1:A:815:ALA:H	2.19	0.45
1:A:922:GLU:HA	1:A:925:ARG:HH21	1.82	0.45
1:B:1179:LEU:O	1:B:1180:ARG:C	2.55	0.45
1:A:1026:PHE:HA	1:A:1090:ARG:NH2	2.32	0.44
1:A:1041:HIS:O	1:A:1043:ASP:N	2.49	0.44
1:B:859:TYR:O	1:B:863:LEU:HG	2.17	0.44
1:B:926:LEU:HD11	1:B:1193:TYR:HE1	1.78	0.44
1:A:807:LEU:HD21	1:A:887:TYR:HB2	1.98	0.44
1:A:811:ARG:NH1	1:A:892:GLU:OE2	2.48	0.44
1:B:779:GLU:O	1:B:781:ALA:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1051:TRP:HB2	1:B:1079:PHE:HE2	1.82	0.44
1:B:1114:SER:HA	1:B:1117:GLN:CG	2.46	0.44
1:B:1153:ILE:HD13	1:B:1187:VAL:HG22	1.98	0.44
1:A:904:LEU:HD13	1:A:1197:TYR:CD1	2.52	0.44
1:A:910:ARG:HB3	1:A:917:SER:CB	2.47	0.44
1:A:1049:GLN:C	1:A:1051:TRP:H	2.20	0.44
1:A:1122:LYS:HB2	1:A:1122:LYS:HZ2	1.82	0.44
1:B:930:ARG:HH21	1:B:1184:LEU:HD11	1.81	0.44
1:B:1085:LYS:O	1:B:1085:LYS:HG2	2.17	0.44
1:A:841:ILE:O	1:A:845:LEU:HG	2.17	0.44
1:A:948:ARG:NH2	1:A:1047:CYS:HA	2.33	0.44
1:A:1026:PHE:HA	1:A:1090:ARG:HH22	1.83	0.44
1:B:831:GLY:CA	1:B:835:THR:HG21	2.47	0.44
1:B:1187:VAL:HA	1:B:1192:GLN:OE1	2.17	0.44
1:A:644:ILE:HG12	1:A:664:TYR:HA	2.00	0.44
1:A:661:ILE:N	1:A:661:ILE:CD1	2.80	0.44
1:A:806:LEU:C	1:A:808:LYS:N	2.71	0.44
1:A:1172:ILE:HD12	1:A:1197:TYR:CE1	2.53	0.44
1:B:869:LEU:O	1:B:869:LEU:HG	2.18	0.44
1:A:687:TYR:CG	1:A:695:ARG:HD2	2.53	0.44
1:A:831:GLY:O	1:A:867:ARG:HD3	2.17	0.44
1:A:922:GLU:HG2	1:A:1173:PHE:HD1	1.83	0.44
1:A:1082:ARG:HD2	1:A:1086:ARG:HA	1.98	0.44
1:B:813:VAL:HA	1:B:816:PHE:CD2	2.52	0.44
1:B:1097:TYR:CD1	1:B:1115:MSE:HG3	2.53	0.44
1:A:845:LEU:HD23	1:A:884:LEU:HD23	2.00	0.44
1:A:1060:ASP:O	1:A:1083:HIS:CB	2.66	0.44
1:B:614:LEU:CD2	1:B:889:GLN:NE2	2.81	0.44
1:B:631:GLU:HG2	1:B:877:TYR:OH	2.18	0.44
1:B:922:GLU:HG2	1:B:1173:PHE:HD1	1.83	0.44
1:B:940:GLN:OE1	1:B:940:GLN:CA	2.60	0.44
1:B:1126:LYS:HB3	1:B:1126:LYS:HZ3	1.82	0.44
1:A:784:ARG:HD2	1:A:820:PHE:CZ	2.53	0.44
1:B:806:LEU:HA	1:B:806:LEU:HD12	1.66	0.44
1:B:806:LEU:O	1:B:809:LEU:HD23	2.18	0.44
1:A:1101:SER:HB3	1:A:1103:GLU:OE1	2.18	0.44
1:B:789:ILE:HG12	1:B:816:PHE:HE2	1.82	0.44
1:B:958:ASN:N	1:B:958:ASN:HD22	2.16	0.44
1:A:832:VAL:HG23	1:A:833:GLY:N	2.33	0.43
1:A:1076:LEU:HG	1:A:1076:LEU:O	2.17	0.43
1:B:912:PRO:HA	1:B:913:PRO:HD2	1.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:LYS:HA	1:B:1090:ARG:NH2	2.33	0.43
1:B:1060:ASP:O	1:B:1083:HIS:CB	2.66	0.43
1:A:689:ASP:N	1:A:866:GLN:HE22	2.17	0.43
1:A:804:HIS:O	1:A:808:LYS:HB2	2.17	0.43
1:B:661:ILE:O	1:B:662:LEU:HD23	2.18	0.43
1:B:748:THR:OG1	1:B:757:LYS:HG3	2.18	0.43
1:B:806:LEU:C	1:B:808:LYS:N	2.69	0.43
1:A:1044:GLN:HE21	1:A:1044:GLN:N	2.16	0.43
1:B:716:TRP:CE2	1:B:776:ASN:HB2	2.53	0.43
1:B:863:LEU:HB3	1:B:870:MSE:HG3	1.99	0.43
1:A:631:GLU:O	1:A:857:TYR:CE1	2.69	0.43
1:A:1070:LYS:HG2	1:A:1075:THR:CB	2.46	0.43
1:B:715:ILE:CD1	1:B:825:VAL:HG21	2.48	0.43
1:B:832:VAL:HG12	1:B:867:ARG:HG2	1.98	0.43
1:A:802:ASP:OD2	1:A:804:HIS:HB3	2.18	0.43
1:A:1055:LYS:O	1:A:1055:LYS:HG2	2.18	0.43
1:A:1123:LEU:HA	1:A:1124:PRO:HD3	1.78	0.43
1:A:697:TYR:CE1	1:A:839:ILE:HG23	2.53	0.43
1:A:873:VAL:CG1	1:A:875:ALA:H	2.20	0.43
1:A:1051:TRP:HB2	1:A:1079:PHE:HE2	1.82	0.43
1:B:802:ASP:OD2	1:B:804:HIS:HB3	2.19	0.43
1:B:806:LEU:HD12	1:B:809:LEU:CD2	2.49	0.43
1:A:691:PHE:O	1:A:692:LYS:HG2	2.19	0.43
1:A:831:GLY:CA	1:A:835:THR:HG21	2.49	0.43
1:B:1028:ARG:HG3	1:B:1028:ARG:NH1	2.34	0.43
1:A:863:LEU:C	1:A:865:ARG:N	2.72	0.43
1:A:1046:ILE:CG2	1:A:1145:ARG:HG2	2.49	0.43
1:A:1082:ARG:HG3	1:A:1089:SER:HA	2.00	0.43
1:B:813:VAL:HG21	1:B:838:TYR:HH	1.81	0.43
1:B:1026:PHE:HA	1:B:1090:ARG:HH22	1.84	0.43
1:A:896:ASN:N	1:A:896:ASN:HD22	2.15	0.43
1:B:614:LEU:HD22	1:B:885:VAL:HG13	2.01	0.43
1:B:949:ASN:C	1:B:949:ASN:ND2	2.71	0.43
1:B:1064:ASP:OD2	1:B:1066:LYS:HE2	2.19	0.43
1:A:599:GLU:CB	1:A:865:ARG:NH2	2.81	0.43
1:A:806:LEU:O	1:A:809:LEU:HD23	2.19	0.43
1:A:1039:LEU:HD23	1:A:1039:LEU:HA	1.87	0.43
1:A:609:HIS:O	1:A:610:ALA:C	2.57	0.42
1:A:660:ASP:C	1:A:661:ILE:HD12	2.38	0.42
1:B:801:GLU:HG2	1:B:1003:LYS:HE3	2.01	0.42
1:B:841:ILE:O	1:B:845:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:ALA:O	1:B:1147:GLY:HA3	2.19	0.42
1:B:1109:PRO:O	1:B:1112:LEU:N	2.50	0.42
1:A:1191:GLU:CD	1:A:1191:GLU:H	2.22	0.42
1:B:777:LYS:HD3	1:B:777:LYS:HA	1.76	0.42
1:B:854:VAL:O	1:B:854:VAL:HG23	2.20	0.42
1:B:962:LEU:HG	1:B:993:ILE:HG22	2.01	0.42
1:B:804:HIS:O	1:B:808:LYS:HB2	2.18	0.42
1:A:789:ILE:HG12	1:A:816:PHE:CE2	2.53	0.42
1:B:708:VAL:HG23	1:B:709:ASP:H	1.84	0.42
1:A:753:ASP:OD1	1:A:778:LYS:HD3	2.19	0.42
1:B:667:ASN:O	1:B:687:TYR:HD1	2.03	0.42
1:B:863:LEU:C	1:B:865:ARG:N	2.73	0.42
1:B:993:ILE:O	1:B:995:ALA:N	2.49	0.42
1:B:1011:GLN:HA	1:B:1144:CYS:O	2.20	0.42
1:B:1018:ILE:HD11	1:B:1049:GLN:H	1.84	0.42
1:B:1040:LYS:HA	1:B:1046:ILE:H	1.85	0.42
1:B:1001:TYR:CE1	1:B:1163:SER:HB3	2.54	0.42
1:B:1007:MSE:SE	1:B:1158:LEU:HD12	2.70	0.42
1:A:828:SER:OG	1:A:835:THR:HG22	2.18	0.42
1:A:1028:ARG:HG3	1:A:1028:ARG:HH11	1.84	0.42
1:A:1083:HIS:NE2	1:A:1085:LYS:HE2	2.35	0.42
1:B:660:ASP:OD2	2:D:2005:SER:N	2.53	0.42
1:B:1039:LEU:CD2	1:B:1048:ALA:O	2.67	0.42
1:B:1039:LEU:CD1	1:B:1049:GLN:HG3	2.48	0.42
1:B:1076:LEU:O	1:B:1076:LEU:HG	2.20	0.42
1:A:736:LYS:HA	1:A:736:LYS:HD3	1.89	0.42
1:A:952:VAL:HG12	1:A:1183:ARG:HH12	1.84	0.42
1:A:599:GLU:N	1:A:641:LYS:HE2	2.35	0.42
1:A:1114:SER:HA	1:A:1117:GLN:CG	2.50	0.42
1:B:876:GLN:O	1:B:880:ILE:HG13	2.20	0.42
1:B:907:MSE:HE2	1:B:922:GLU:OE1	2.20	0.42
1:B:939:ASN:HA	1:B:944:LYS:HD3	2.00	0.42
1:B:1001:TYR:HE2	1:B:1166:THR:HG1	1.65	0.42
1:B:1148:SER:OG	1:B:1183:ARG:HD3	2.20	0.42
1:A:614:LEU:HD22	1:A:885:VAL:HG13	2.01	0.42
1:B:657:ARG:HH12	1:B:704:ARG:HA	1.85	0.42
1:B:911:ASP:CB	1:B:912:PRO:CD	2.94	0.42
1:B:1153:ILE:HD11	1:B:1192:GLN:CB	2.37	0.42
1:A:924:GLN:HA	1:A:924:GLN:NE2	2.35	0.41
1:B:806:LEU:C	1:B:808:LYS:H	2.24	0.41
1:A:902:PRO:O	1:A:905:HIS:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:LYS:CE	1:A:1027:GLN:HB3	2.46	0.41
1:A:1167:GLU:O	1:A:1168:GLU:HB2	2.20	0.41
1:A:761:HIS:HE1	1:A:763:ARG:CZ	2.34	0.41
1:A:932:TRP:CH2	1:A:933:ARG:NE	2.88	0.41
1:A:954:PRO:HD3	1:A:994:ASN:OD1	2.20	0.41
1:A:1034:VAL:HG12	1:A:1036:LEU:HD13	2.02	0.41
1:B:723:ILE:O	1:B:789:ILE:HD12	2.20	0.41
1:B:813:VAL:C	1:B:815:ALA:N	2.74	0.41
1:B:864:ARG:HD2	1:B:870:MSE:HB2	2.02	0.41
1:A:806:LEU:HA	1:A:809:LEU:CD2	2.50	0.41
1:A:930:ARG:CG	1:A:931:SER:N	2.83	0.41
1:A:1019:GLY:O	1:A:1023:GLN:OE1	2.37	0.41
1:B:811:ARG:HD2	1:B:892:GLU:HG3	2.02	0.41
1:B:947:ASN:CG	1:B:994:ASN:HD22	2.24	0.41
1:B:1128:SER:O	1:B:1129:SER:CB	2.67	0.41
1:A:708:VAL:HG23	1:A:709:ASP:N	2.35	0.41
1:A:789:ILE:CG1	1:A:816:PHE:CE2	2.98	0.41
1:A:890:PHE:HE2	1:A:927:PRO:HD3	1.81	0.41
1:A:1028:ARG:N	1:A:1028:ARG:HD2	2.34	0.41
1:B:726:VAL:O	1:B:727:THR:HB	2.19	0.41
1:A:831:GLY:C	1:A:835:THR:HG21	2.41	0.41
1:A:1061:ILE:C	1:A:1061:ILE:CD1	2.89	0.41
1:B:801:GLU:OE1	1:B:805:LEU:HD11	2.21	0.41
1:A:832:VAL:HG12	1:A:867:ARG:HG2	2.02	0.41
1:A:863:LEU:HD22	1:A:870:MSE:HE2	2.02	0.41
1:A:887:TYR:O	1:A:891:GLY:HA2	2.21	0.41
1:A:894:GLU:HG2	1:A:1169:VAL:HG22	2.03	0.41
1:B:728:ARG:HH21	1:B:792:THR:HB	1.85	0.41
1:B:1006:VAL:HG12	1:B:1007:MSE:N	2.34	0.41
1:A:726:VAL:O	1:A:727:THR:HB	2.21	0.41
1:A:1015:LYS:HB3	1:A:1015:LYS:HZ3	1.86	0.41
1:A:1111:GLU:HA	1:A:1114:SER:OG	2.21	0.41
1:B:624:GLU:OE2	1:B:624:GLU:O	2.39	0.41
1:B:1123:LEU:HB2	1:B:1124:PRO:CD	2.51	0.41
1:B:1180:ARG:HH11	1:B:1180:ARG:HG2	1.86	0.41
1:A:906:ASN:O	1:A:909:LYS:HG3	2.21	0.41
1:A:1013:PRO:HD2	1:A:1047:CYS:SG	2.61	0.41
1:A:1017:THR:C	1:A:1019:GLY:H	2.24	0.41
1:B:908:LYS:O	1:B:917:SER:CB	2.68	0.41
1:B:1133:LYS:HG3	1:B:1134:HIS:N	2.35	0.41
1:A:659:VAL:HG22	1:A:659:VAL:O	2.22	0.40

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:HIS:N	1:A:956:ASP:OD2	2.47	0.40
1:A:1006:VAL:HG12	1:A:1007:MSE:N	2.36	0.40
1:A:960:VAL:HG23	1:A:995:ALA:O	2.22	0.40
1:B:608:ILE:HG21	1:B:613:LEU:HA	2.02	0.40
1:B:734:ARG:HH11	1:B:734:ARG:HB3	1.86	0.40
1:B:807:LEU:HD21	1:B:887:TYR:HB2	2.01	0.40
1:B:845:LEU:HD23	1:B:884:LEU:HD23	2.03	0.40
1:B:934:THR:OG1	1:B:956:ASP:HB2	2.21	0.40
1:B:1034:VAL:HG12	1:B:1036:LEU:CD1	2.52	0.40
1:A:661:ILE:O	1:A:662:LEU:HD23	2.22	0.40
1:A:716:TRP:CE2	1:A:776:ASN:HB2	2.56	0.40
1:A:932:TRP:CZ2	1:A:1181:LYS:HG2	2.57	0.40
1:B:651:PHE:O	1:B:655:LYS:HE3	2.21	0.40
1:A:1060:ASP:O	1:A:1083:HIS:HB3	2.21	0.40
1:A:1107:ALA:C	1:A:1109:PRO:HD3	2.42	0.40
1:A:1110:LYS:HG2	1:A:1111:GLU:N	2.37	0.40
1:B:873:VAL:O	1:B:877:TYR:N	2.49	0.40
1:B:1122:LYS:HB2	1:B:1122:LYS:HZ2	1.85	0.40
1:A:1018:ILE:HD11	1:A:1049:GLN:H	1.85	0.40
1:A:1025:ILE:HD11	1:A:1081:LEU:HD11	2.02	0.40
1:A:1046:ILE:HG23	1:A:1145:ARG:CG	2.50	0.40
1:B:643:PRO:O	1:B:665:ASP:HB2	2.21	0.40
1:B:910:ARG:O	1:B:911:ASP:C	2.60	0.40
1:B:938:GLY:HA2	1:B:992:TYR:CZ	2.56	0.40
1:B:991:LYS:HD3	1:B:991:LYS:N	2.36	0.40
1:B:1017:THR:C	1:B:1019:GLY:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	565/610 (93%)	461 (82%)	80 (14%)	24 (4%)	3	10
1	B	578/610 (95%)	451 (78%)	93 (16%)	34 (6%)	1	5
2	C	1/4 (25%)	1 (100%)	0	0	100	100
2	D	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1145/1228 (93%)	914 (80%)	173 (15%)	58 (5%)	2	7

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	819	PHE
1	A	870	MSE
1	A	871	VAL
1	A	911	ASP
1	A	930	ARG
1	A	1050	TYR
1	A	1086	ARG
1	A	1099	ASN
1	A	1187	VAL
1	B	870	MSE
1	B	871	VAL
1	B	895	VAL
1	B	911	ASP
1	B	930	ARG
1	B	1050	TYR
1	B	1086	ARG
1	B	1099	ASN
1	B	1123	LEU
1	B	1124	PRO
1	B	1129	SER
1	B	1132	ASN
1	B	1133	LYS
1	B	1186	MSE
1	A	610	ALA
1	A	833	GLY
1	A	1042	GLY
1	A	1056	GLN
1	A	1084	SER
1	B	833	GLY
1	B	941	GLU
1	B	1042	GLY
1	B	1056	GLN
1	B	1084	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1145	ARG
1	A	932	TRP
1	A	941	GLU
1	A	959	ARG
1	A	1015	LYS
1	A	1089	SER
1	A	1145	ARG
1	B	610	ALA
1	B	780	LYS
1	B	932	TRP
1	B	1018	ILE
1	B	1048	ALA
1	B	1089	SER
1	A	1018	ILE
1	B	915	GLU
1	B	991	LYS
1	B	1015	LYS
1	B	1149	GLN
1	A	1048	ALA
1	B	1102	VAL
1	A	903	TYR
1	A	1102	VAL
1	B	913	PRO
1	B	747	GLY
1	B	1138	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	514/538 (96%)	458 (89%)	56 (11%)	6	19
1	B	524/538 (97%)	461 (88%)	63 (12%)	5	15
2	C	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	1044/1082 (96%)	924 (88%)	120 (12%)	5	17

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	602	LEU
1	A	611	ASP
1	A	614	LEU
1	A	629	LEU
1	A	637	ARG
1	A	641	LYS
1	A	665	ASP
1	A	673	GLU
1	A	721	THR
1	A	734	ARG
1	A	782	THR
1	A	785	GLU
1	A	789	ILE
1	A	792	THR
1	A	806	LEU
1	A	835	THR
1	A	848	LEU
1	A	864	ARG
1	A	872	GLN
1	A	874	GLU
1	A	879	LEU
1	A	909	LYS
1	A	910	ARG
1	A	911	ASP
1	A	919	LEU
1	A	925	ARG
1	A	940	GLN
1	A	949	ASN
1	A	951	ASN
1	A	957	TYR
1	A	958	ASN
1	A	991	LYS
1	A	1025	ILE
1	A	1028	ARG
1	A	1036	LEU
1	A	1043	ASP
1	A	1044	GLN
1	A	1049	GLN
1	A	1056	GLN
1	A	1065	LEU
1	A	1075	THR
1	A	1076	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1083	HIS
1	A	1087	LYS
1	A	1091	THR
1	A	1104	GLN
1	A	1110	LYS
1	A	1114	SER
1	A	1115	MSE
1	A	1121	GLN
1	A	1122	LYS
1	A	1125	GLN
1	A	1150	GLN
1	A	1169	VAL
1	A	1180	ARG
1	A	1184	LEU
1	B	602	LEU
1	B	611	ASP
1	B	614	LEU
1	B	629	LEU
1	B	637	ARG
1	B	641	LYS
1	B	665	ASP
1	B	673	GLU
1	B	721	THR
1	B	734	ARG
1	B	778	LYS
1	B	782	THR
1	B	785	GLU
1	B	789	ILE
1	B	792	THR
1	B	806	LEU
1	B	820	PHE
1	B	835	THR
1	B	848	LEU
1	B	864	ARG
1	B	872	GLN
1	B	874	GLU
1	B	879	LEU
1	B	888	ASN
1	B	896	ASN
1	B	909	LYS
1	B	919	LEU
1	B	925	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	930	ARG
1	B	940	GLN
1	B	949	ASN
1	B	951	ASN
1	B	957	TYR
1	B	958	ASN
1	B	991	LYS
1	B	992	TYR
1	B	1025	ILE
1	B	1028	ARG
1	B	1036	LEU
1	B	1043	ASP
1	B	1044	GLN
1	B	1049	GLN
1	B	1056	GLN
1	B	1058	TYR
1	B	1065	LEU
1	B	1075	THR
1	B	1076	LEU
1	B	1083	HIS
1	B	1087	LYS
1	B	1091	THR
1	B	1104	GLN
1	B	1114	SER
1	B	1121	GLN
1	B	1122	LYS
1	B	1124	PRO
1	B	1125	GLN
1	B	1126	LYS
1	B	1130	GLU
1	B	1132	ASN
1	B	1150	GLN
1	B	1169	VAL
1	B	1180	ARG
1	B	1184	LEU
2	C	2003	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	604	ASN
1	A	633	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	652	ASN
1	A	653	GLN
1	A	718	GLN
1	A	761	HIS
1	A	770	GLN
1	A	866	GLN
1	A	881	HIS
1	A	889	GLN
1	A	896	ASN
1	A	924	GLN
1	A	943	ASN
1	A	947	ASN
1	A	949	ASN
1	A	951	ASN
1	A	958	ASN
1	A	1044	GLN
1	A	1049	GLN
1	A	1094	GLN
1	A	1117	GLN
1	A	1121	GLN
1	A	1149	GLN
1	A	1150	GLN
1	B	604	ASN
1	B	633	GLN
1	B	652	ASN
1	B	653	GLN
1	B	718	GLN
1	B	761	HIS
1	B	770	GLN
1	B	818	ASN
1	B	866	GLN
1	B	881	HIS
1	B	889	GLN
1	B	906	ASN
1	B	924	GLN
1	B	943	ASN
1	B	947	ASN
1	B	949	ASN
1	B	951	ASN
1	B	958	ASN
1	B	994	ASN
1	B	1044	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1049	GLN
1	B	1094	GLN
1	B	1117	GLN
1	B	1121	GLN
1	B	1125	GLN
1	B	1132	ASN
1	B	1149	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PTR	D	2004	2	15,16,17	1.89	5 (33%)	19,22,24	2.97	8 (42%)
2	PTR	C	2004	2	15,16,17	1.81	5 (33%)	19,22,24	2.44	7 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	D	2004	2	1/1/2/3	3/10/11/13	0/1/1/1
2	PTR	C	2004	2	1/1/2/3	3/10/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2004	PTR	P-OH	4.28	1.65	1.59
2	C	2004	PTR	P-OH	3.81	1.65	1.59
2	C	2004	PTR	OH-CZ	2.88	1.47	1.40
2	D	2004	PTR	OH-CZ	2.87	1.47	1.40
2	C	2004	PTR	P-O3P	-2.61	1.44	1.54
2	D	2004	PTR	P-O3P	-2.56	1.45	1.54
2	C	2004	PTR	CE2-CD2	2.30	1.42	1.38
2	D	2004	PTR	CE2-CD2	2.24	1.42	1.38
2	D	2004	PTR	CD2-CG	2.21	1.43	1.38
2	C	2004	PTR	CD2-CG	2.16	1.43	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2004	PTR	CB-CA-C	7.47	125.48	111.47
2	C	2004	PTR	CB-CA-C	6.18	123.06	111.47
2	D	2004	PTR	OH-CZ-CE2	5.80	136.48	119.23
2	D	2004	PTR	OH-CZ-CE1	-5.59	102.61	119.23
2	C	2004	PTR	OH-CZ-CE2	4.61	132.95	119.23
2	C	2004	PTR	OH-CZ-CE1	-4.30	106.43	119.23
2	D	2004	PTR	CG-CB-CA	3.57	121.33	114.10
2	C	2004	PTR	CG-CB-CA	3.33	120.84	114.10
2	D	2004	PTR	P-OH-CZ	3.11	133.71	123.75
2	D	2004	PTR	CE2-CD2-CG	-2.31	117.85	121.03
2	D	2004	PTR	CB-CG-CD1	-2.24	116.46	120.91
2	D	2004	PTR	O3P-P-O2P	2.15	115.85	107.64
2	C	2004	PTR	CE2-CD2-CG	-2.13	118.10	121.03
2	C	2004	PTR	O3P-P-OH	2.03	111.59	105.24
2	C	2004	PTR	CB-CG-CD1	-2.01	116.92	120.91

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2004	PTR	CA
2	D	2004	PTR	CA

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2004	PTR	C-CA-CB-CG
2	D	2004	PTR	C-CA-CB-CG
2	D	2004	PTR	CA-CB-CG-CD2
2	D	2004	PTR	CA-CB-CG-CD1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	2004	PTR	CA-CB-CG-CD2
2	C	2004	PTR	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2004	PTR	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.